



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:56 am GMT

PDB ID : 1F1H  
Title : CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM  
SALMONELLA TYPHIMURIUM WITH THALLIUM IONS  
Authors : Gill, H.S.; Eisenberg, D.  
Deposited on : 2000-05-19  
Resolution : 2.67 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

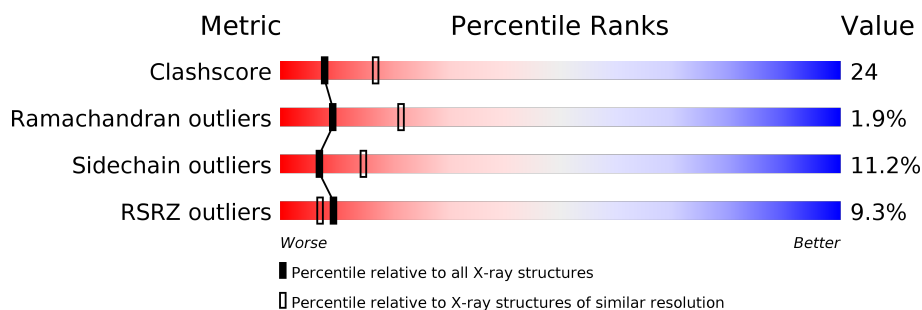
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3418 (2.70-2.66)
Ramachandran outliers	110173	3367 (2.70-2.66)
Sidechain outliers	110143	3367 (2.70-2.66)
RSRZ outliers	101464	3069 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	468	<div> <div>17%</div> <div>69%</div> <div>23%</div> <div>7%</div> <div>.</div> </div>
1	B	468	<div> <div>11%</div> <div>71%</div> <div>21%</div> <div>7%</div> <div>.</div> </div>
1	C	468	<div> <div>10%</div> <div>69%</div> <div>23%</div> <div>7%</div> <div>.</div> </div>
1	D	468	<div> <div>8%</div> <div>70%</div> <div>22%</div> <div>7%</div> <div>.</div> </div>
1	E	468	<div> <div>12%</div> <div>70%</div> <div>22%</div> <div>7%</div> <div>.</div> </div>
1	F	468	<div> <div>9%</div> <div>70%</div> <div>23%</div> <div>7%</div> <div>.</div> </div>
1	G	468	<div> <div>8%</div> <div>71%</div> <div>22%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	468	
1	I	468	
1	J	468	
1	K	468	
1	L	468	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	B	1472	-	-	-	X
3	ADP	D	1474	-	-	-	X
3	ADP	F	1476	-	-	-	X
3	ADP	I	1479	-	-	-	X
3	ADP	K	1481	-	-	-	X
3	ADP	L	1482	-	-	-	X
5	MPD	A	1483	-	-	X	X
5	MPD	B	1484	-	-	X	X
5	MPD	C	1485	-	-	X	X
5	MPD	D	1486	-	-	X	X
5	MPD	E	1487	-	-	X	X
5	MPD	F	1488	-	-	X	X
5	MPD	G	1489	-	-	X	X
5	MPD	H	1490	-	-	X	X
5	MPD	I	1491	-	-	X	X
5	MPD	J	1492	-	-	X	X
5	MPD	K	1493	-	-	X	X
5	MPD	L	1494	-	-	X	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 45564 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN (GLUTAMINE SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	B	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	C	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	D	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	E	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	F	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	G	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	H	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	I	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	J	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	K	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	L	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

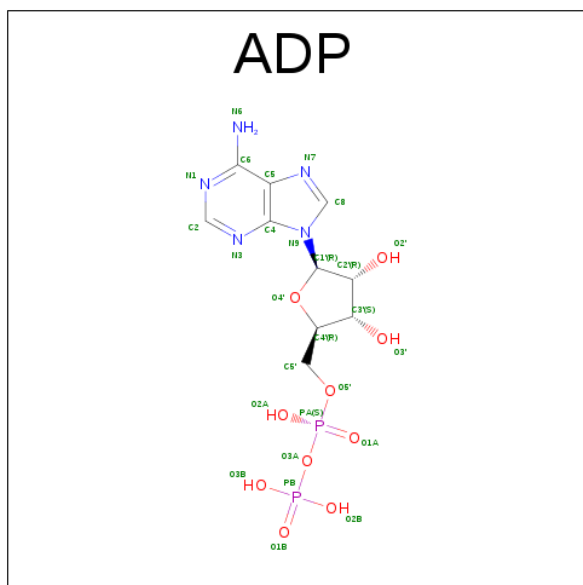
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mn	0	0
			2	2		
2	K	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	H	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	I	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	L	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is THALLIUM (I) ION (three-letter code: TL) (formula: Tl).

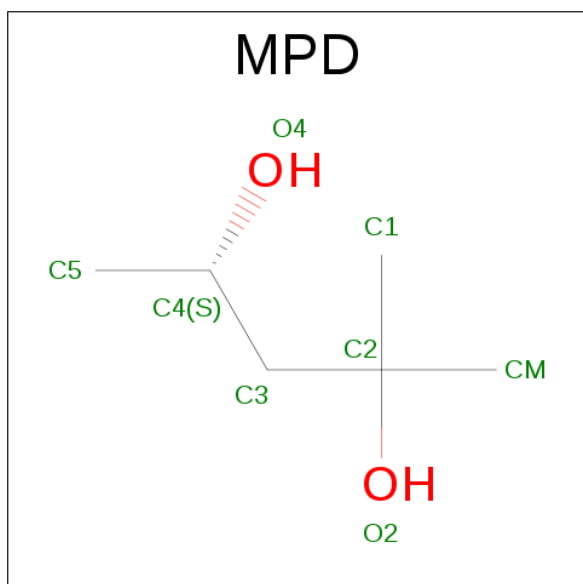
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Tl	0	0
			2	2		
4	J	2	Total	Tl	0	0
			2	2		
4	D	2	Total	Tl	0	0
			2	2		
4	K	2	Total	Tl	0	0
			2	2		
4	E	2	Total	Tl	0	0
			2	2		
4	H	2	Total	Tl	0	0
			2	2		
4	B	2	Total	Tl	0	0
			2	2		
4	I	2	Total	Tl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	Tl 2	0	0
4	A	2	Total 2	Tl 2	0	0
4	L	2	Total 2	Tl 2	0	0
4	F	2	Total 2	Tl 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 8	C 6	O 2	0	0
5	B	1	Total 8	C 6	O 2	0	0
5	C	1	Total 8	C 6	O 2	0	0
5	D	1	Total 8	C 6	O 2	0	0
5	E	1	Total 8	C 6	O 2	0	0
5	F	1	Total 8	C 6	O 2	0	0
5	G	1	Total 8	C 6	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			8	6	2		
5	I	1	Total	C	O	0	0
			8	6	2		
5	J	1	Total	C	O	0	0
			8	6	2		
5	K	1	Total	C	O	0	0
			8	6	2		
5	L	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

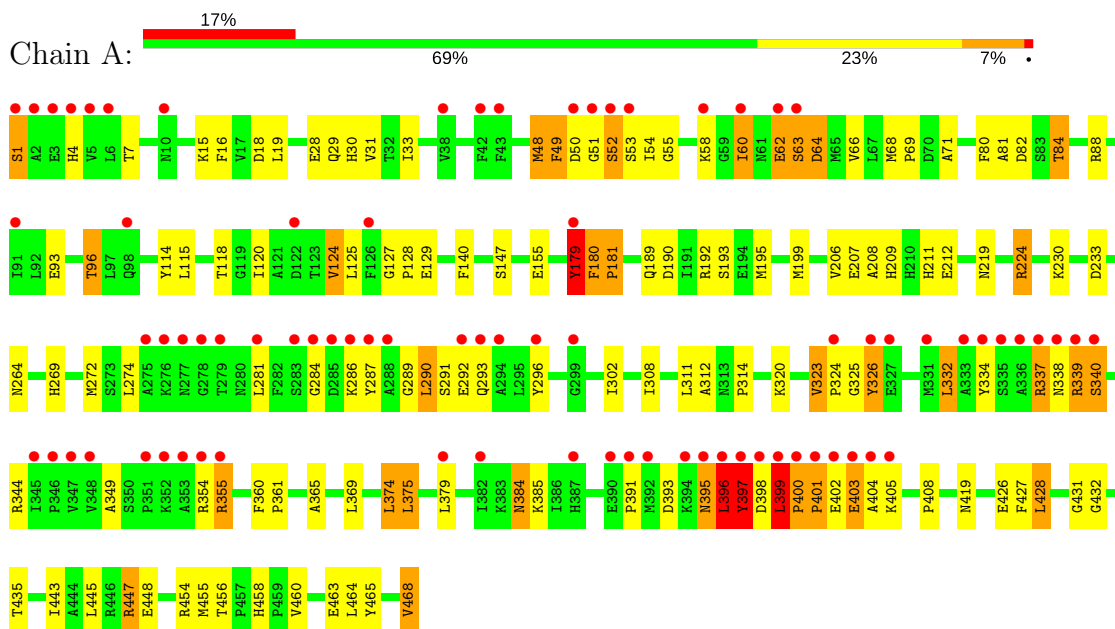
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	120	Total	O	0	0
			120	120		
6	B	121	Total	O	0	0
			121	121		
6	C	119	Total	O	0	0
			119	119		
6	D	122	Total	O	0	0
			122	122		
6	E	122	Total	O	0	0
			122	122		
6	F	121	Total	O	0	0
			121	121		
6	G	122	Total	O	0	0
			122	122		
6	H	121	Total	O	0	0
			121	121		
6	I	122	Total	O	0	0
			122	122		
6	J	120	Total	O	0	0
			120	120		
6	K	123	Total	O	0	0
			123	123		
6	L	119	Total	O	0	0
			119	119		



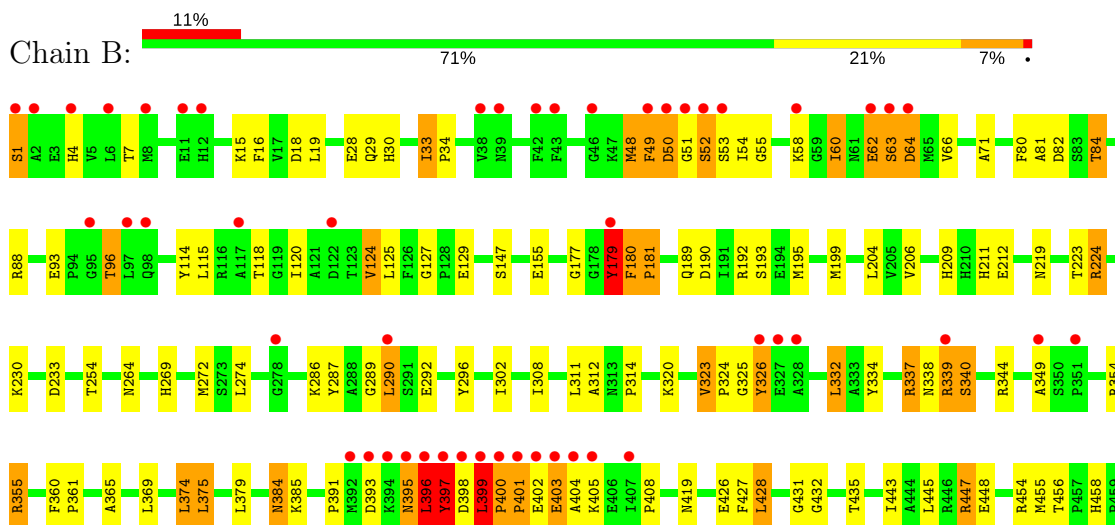
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

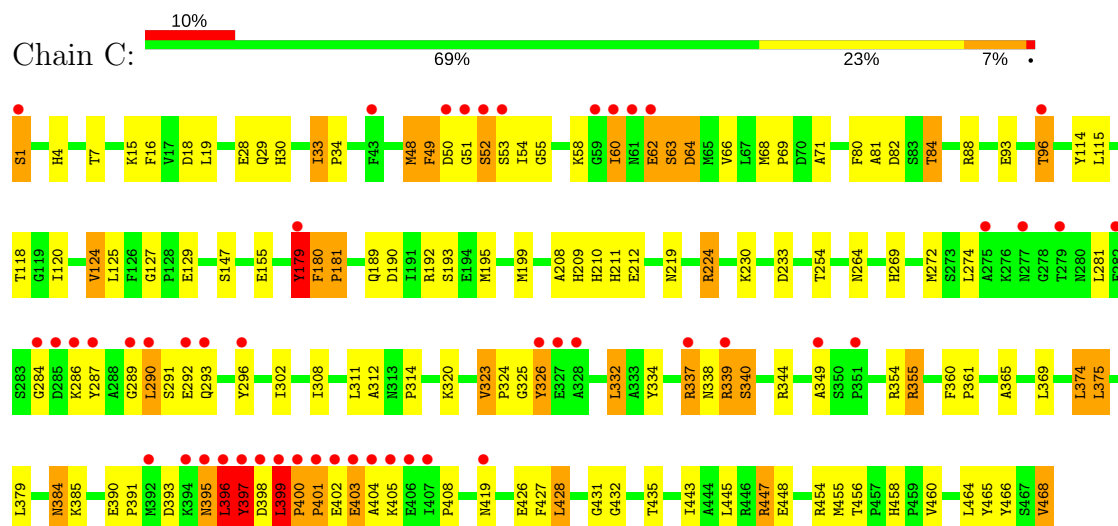


#### • Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

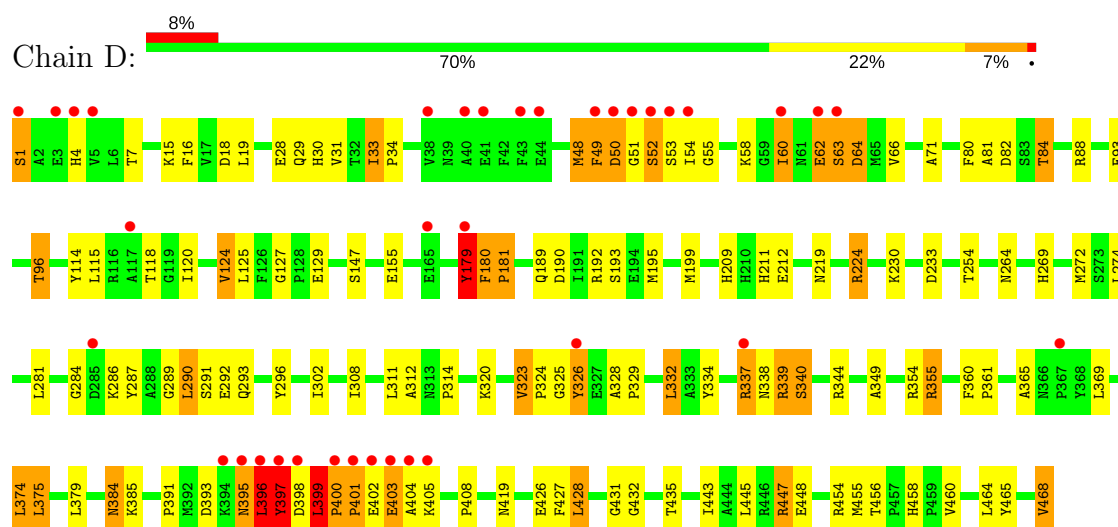




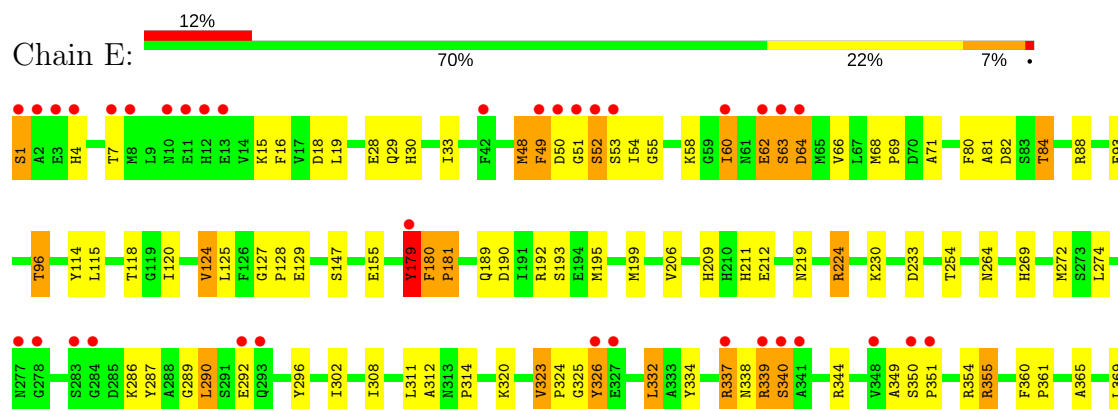
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



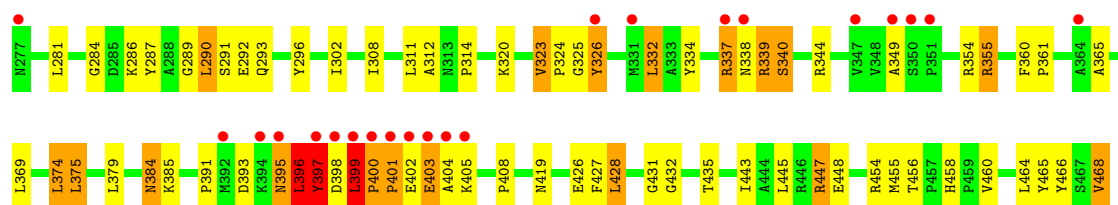
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



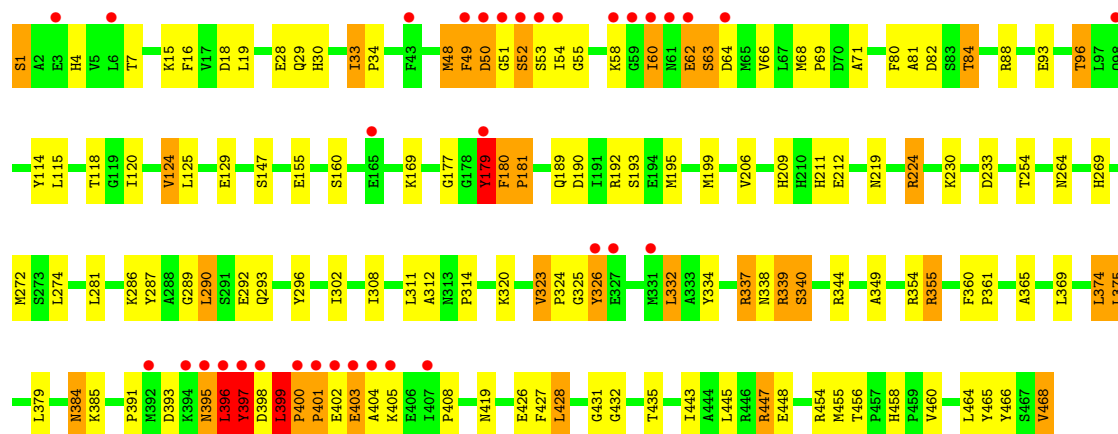
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



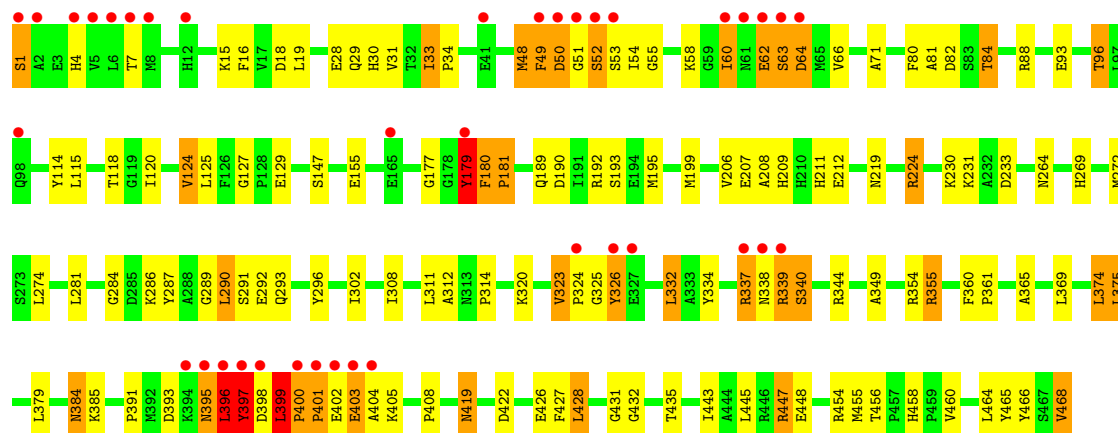




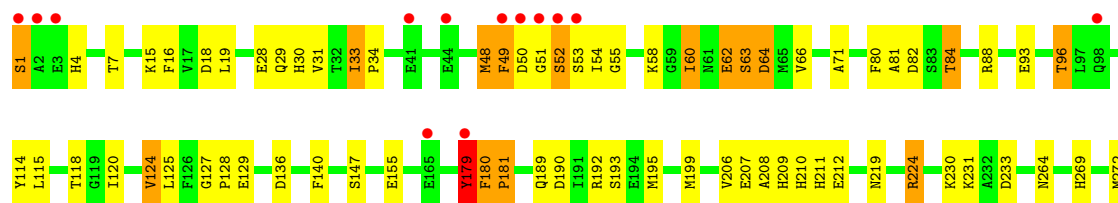
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

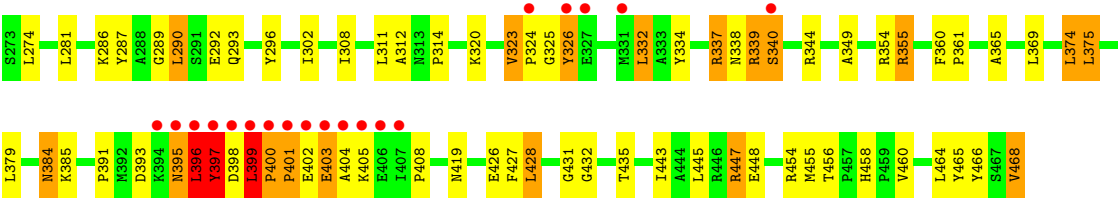


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

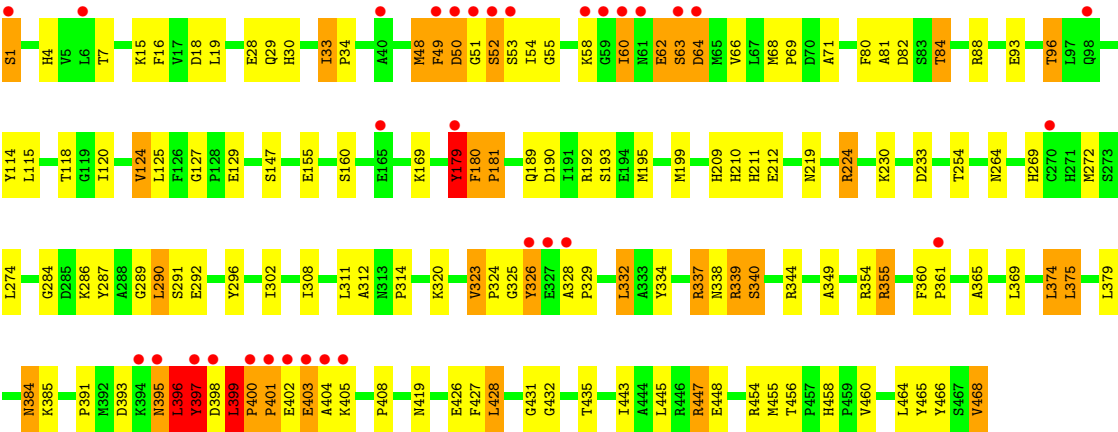


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)





• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.13Å 132.79Å 196.78Å 90.00° 102.44° 90.00°	Depositor
Resolution (Å)	32.00 – 2.67 36.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.0 (32.00-2.67) 82.0 (36.87-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.68Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.232 , 0.263 0.231 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 60.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	45564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, MN, TL, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.52	0/3724	0.85	4/5043 (0.1%)
1	B	0.52	0/3724	0.85	4/5043 (0.1%)
1	C	0.52	0/3724	0.85	4/5043 (0.1%)
1	D	0.52	0/3724	0.85	4/5043 (0.1%)
1	E	0.52	0/3724	0.85	4/5043 (0.1%)
1	F	0.52	0/3724	0.85	4/5043 (0.1%)
1	G	0.52	0/3724	0.85	4/5043 (0.1%)
1	H	0.52	0/3724	0.85	4/5043 (0.1%)
1	I	0.52	0/3724	0.85	4/5043 (0.1%)
1	J	0.52	0/3724	0.85	4/5043 (0.1%)
1	K	0.52	0/3724	0.85	4/5043 (0.1%)
1	L	0.52	0/3724	0.85	4/5043 (0.1%)
All	All	0.52	0/44688	0.85	48/60516 (0.1%)

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	179	TYR	CB-CG-CD1	6.17	124.70	121.00
1	K	179	TYR	CB-CG-CD1	6.14	124.69	121.00
1	J	179	TYR	CB-CG-CD1	6.12	124.67	121.00
1	D	179	TYR	CB-CG-CD1	6.11	124.67	121.00
1	I	179	TYR	CB-CG-CD1	6.10	124.66	121.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3637	0	3542	186	0
1	B	3637	0	3543	185	0
1	C	3637	0	3543	188	0
1	D	3637	0	3542	180	0
1	E	3637	0	3543	175	0
1	F	3637	0	3543	176	0
1	G	3637	0	3542	176	0
1	H	3637	0	3543	180	0
1	I	3637	0	3542	189	0
1	J	3637	0	3543	193	0
1	K	3637	0	3543	189	0
1	L	3637	0	3543	179	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	27	0	10	4	0
3	B	27	0	10	4	0
3	C	27	0	10	4	0
3	D	27	0	10	4	0
3	E	27	0	10	4	0
3	F	27	0	10	4	0
3	G	27	0	10	4	0
3	H	27	0	10	4	0
3	I	27	0	10	3	0
3	J	27	0	10	4	0
3	K	27	0	10	4	0
3	L	27	0	10	4	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	8	0	14	29	0
5	B	8	0	14	34	0
5	C	8	0	14	33	0
5	D	8	0	14	34	0
5	E	8	0	14	29	0
5	F	8	0	14	34	0
5	G	8	0	14	31	0
5	H	8	0	14	33	0
5	I	8	0	14	35	0
5	J	8	0	14	34	0
5	K	8	0	14	33	0
5	L	8	0	14	32	0
6	A	120	0	0	6	0
6	B	121	0	0	6	0
6	C	119	0	0	5	0
6	D	122	0	0	6	0
6	E	122	0	0	6	0
6	F	121	0	0	5	0
6	G	122	0	0	6	0
6	H	121	0	0	5	0
6	I	122	0	0	6	0
6	J	120	0	0	6	0
6	K	123	0	0	6	0
6	L	119	0	0	6	0
All	All	45564	0	42800	2077	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 2077 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1481:ADP:N9	3:K:1481:ADP:C1'	1.71	1.54
3:I:1479:ADP:N9	3:I:1479:ADP:C1'	1.71	1.54
3:B:1472:ADP:N9	3:B:1472:ADP:C1'	1.71	1.52
3:F:1476:ADP:N9	3:F:1476:ADP:C1'	1.71	1.52
3:E:1475:ADP:N9	3:E:1475:ADP:C1'	1.71	1.51

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
1	B	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
1	C	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
1	D	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
1	E	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
1	F	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
1	G	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
1	H	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
1	I	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
1	J	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
1	K	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
1	L	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	9	21
All	All	5592/5616 (100%)	5148 (92%)	336 (6%)	108 (2%)	9	21

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	SER

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Mol	Chain	Res	Type
1	A	62	GLU
1	A	180	PHE
1	A	399	LEU
1	A	400	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/384 (100%)	341 (89%)	43 (11%)	7	15
1	B	384/384 (100%)	341 (89%)	43 (11%)	7	15
1	C	384/384 (100%)	341 (89%)	43 (11%)	7	15
1	D	384/384 (100%)	341 (89%)	43 (11%)	7	15
1	E	384/384 (100%)	341 (89%)	43 (11%)	7	15
1	F	384/384 (100%)	341 (89%)	43 (11%)	7	15
1	G	384/384 (100%)	341 (89%)	43 (11%)	7	15
1	H	384/384 (100%)	341 (89%)	43 (11%)	7	15
1	I	384/384 (100%)	341 (89%)	43 (11%)	7	15
1	J	384/384 (100%)	341 (89%)	43 (11%)	7	15
1	K	384/384 (100%)	341 (89%)	43 (11%)	7	15
1	L	384/384 (100%)	341 (89%)	43 (11%)	7	15
All	All	4608/4608 (100%)	4092 (89%)	516 (11%)	7	15

5 of 516 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	181	PRO
1	G	355	ARG
1	L	33	ILE
1	F	332	LEU
1	G	48	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	244	ASN
1	G	395	ASN
1	L	211	HIS
1	F	338	ASN
1	G	211	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 48 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ADP	A	1471	-	25,29,29	2.70	9 (36%)	24,45,45	3.35	8 (33%)
5	MPD	A	1483	-	7,7,7	1.08	0	9,10,10	0.69	0
3	ADP	B	1472	-	25,29,29	2.70	9 (36%)	24,45,45	3.36	8 (33%)
5	MPD	B	1484	-	7,7,7	1.08	0	9,10,10	0.69	0
3	ADP	C	1473	-	25,29,29	2.70	9 (36%)	24,45,45	3.35	8 (33%)
5	MPD	C	1485	-	7,7,7	1.09	0	9,10,10	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	D	1474	-	25,29,29	2.70	9 (36%)	24,45,45	3.35	8 (33%)
5	MPD	D	1486	-	7,7,7	1.07	0	9,10,10	0.69	0
3	ADP	E	1475	-	25,29,29	2.70	9 (36%)	24,45,45	3.35	8 (33%)
5	MPD	E	1487	-	7,7,7	1.07	0	9,10,10	0.69	0
3	ADP	F	1476	-	25,29,29	2.70	9 (36%)	24,45,45	3.35	8 (33%)
5	MPD	F	1488	-	7,7,7	1.08	0	9,10,10	0.69	0
3	ADP	G	1477	-	25,29,29	2.71	9 (36%)	24,45,45	3.35	8 (33%)
5	MPD	G	1489	-	7,7,7	1.07	0	9,10,10	0.69	0
3	ADP	H	1478	-	25,29,29	2.71	9 (36%)	24,45,45	3.36	8 (33%)
5	MPD	H	1490	-	7,7,7	1.08	0	9,10,10	0.69	0
3	ADP	I	1479	-	25,29,29	2.70	9 (36%)	24,45,45	3.36	8 (33%)
5	MPD	I	1491	-	7,7,7	1.08	0	9,10,10	0.69	0
3	ADP	J	1480	-	25,29,29	2.70	9 (36%)	24,45,45	3.36	8 (33%)
5	MPD	J	1492	-	7,7,7	1.07	0	9,10,10	0.69	0
3	ADP	K	1481	-	25,29,29	2.71	9 (36%)	24,45,45	3.35	8 (33%)
5	MPD	K	1493	-	7,7,7	1.07	0	9,10,10	0.69	0
3	ADP	L	1482	-	25,29,29	2.71	9 (36%)	24,45,45	3.36	8 (33%)
5	MPD	L	1494	-	7,7,7	1.08	0	9,10,10	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	1471	-	-	0/12/32/32	0/3/3/3
5	MPD	A	1483	-	-	0/5/5/5	0/0/0/0
3	ADP	B	1472	-	-	0/12/32/32	0/3/3/3
5	MPD	B	1484	-	-	0/5/5/5	0/0/0/0
3	ADP	C	1473	-	-	0/12/32/32	0/3/3/3
5	MPD	C	1485	-	-	0/5/5/5	0/0/0/0
3	ADP	D	1474	-	-	0/12/32/32	0/3/3/3
5	MPD	D	1486	-	-	0/5/5/5	0/0/0/0
3	ADP	E	1475	-	-	0/12/32/32	0/3/3/3
5	MPD	E	1487	-	-	0/5/5/5	0/0/0/0
3	ADP	F	1476	-	-	0/12/32/32	0/3/3/3
5	MPD	F	1488	-	-	0/5/5/5	0/0/0/0
3	ADP	G	1477	-	-	0/12/32/32	0/3/3/3
5	MPD	G	1489	-	-	0/5/5/5	0/0/0/0
3	ADP	H	1478	-	-	0/12/32/32	0/3/3/3
5	MPD	H	1490	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	I	1479	-	-	0/12/32/32	0/3/3/3
5	MPD	I	1491	-	-	0/5/5/5	0/0/0/0
3	ADP	J	1480	-	-	0/12/32/32	0/3/3/3
5	MPD	J	1492	-	-	0/5/5/5	0/0/0/0
3	ADP	K	1481	-	-	0/12/32/32	0/3/3/3
5	MPD	K	1493	-	-	0/5/5/5	0/0/0/0
3	ADP	L	1482	-	-	0/12/32/32	0/3/3/3
5	MPD	L	1494	-	-	0/5/5/5	0/0/0/0

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1478	ADP	C3'-C4'	-2.67	1.46	1.53
3	J	1480	ADP	C3'-C4'	-2.66	1.46	1.53
3	K	1481	ADP	C3'-C4'	-2.66	1.46	1.53
3	G	1477	ADP	C3'-C4'	-2.66	1.46	1.53
3	L	1482	ADP	C3'-C4'	-2.66	1.46	1.53

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1478	ADP	C4'-O4'-C1'	-8.97	100.22	109.77
3	L	1482	ADP	C4'-O4'-C1'	-8.96	100.24	109.77
3	I	1479	ADP	C4'-O4'-C1'	-8.95	100.24	109.77
3	J	1480	ADP	C4'-O4'-C1'	-8.93	100.27	109.77
3	B	1472	ADP	C4'-O4'-C1'	-8.92	100.28	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 438 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1471	ADP	4	0
5	A	1483	MPD	29	0
3	B	1472	ADP	4	0
5	B	1484	MPD	34	0
3	C	1473	ADP	4	0
5	C	1485	MPD	33	0
3	D	1474	ADP	4	0
5	D	1486	MPD	34	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1475	ADP	4	0
5	E	1487	MPD	29	0
3	F	1476	ADP	4	0
5	F	1488	MPD	34	0
3	G	1477	ADP	4	0
5	G	1489	MPD	31	0
3	H	1478	ADP	4	0
5	H	1490	MPD	33	0
3	I	1479	ADP	3	0
5	I	1491	MPD	35	0
3	J	1480	ADP	4	0
5	J	1492	MPD	34	0
3	K	1481	ADP	4	0
5	K	1493	MPD	33	0
3	L	1482	ADP	4	0
5	L	1494	MPD	32	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	468/468 (100%)	0.64	79 (16%) 2 1	18, 39, 91, 100	29 (6%)
1	B	468/468 (100%)	0.40	50 (10%) 7 5	18, 39, 91, 100	29 (6%)
1	C	468/468 (100%)	0.30	48 (10%) 7 5	18, 39, 91, 100	29 (6%)
1	D	468/468 (100%)	0.14	36 (7%) 14 12	18, 39, 91, 100	29 (6%)
1	E	468/468 (100%)	0.35	56 (11%) 5 3	18, 39, 91, 100	29 (6%)
1	F	468/468 (100%)	0.31	43 (9%) 10 7	18, 39, 91, 100	29 (6%)
1	G	468/468 (100%)	0.25	37 (7%) 13 11	18, 39, 91, 100	29 (6%)
1	H	468/468 (100%)	0.32	37 (7%) 13 11	18, 39, 91, 100	29 (6%)
1	I	468/468 (100%)	0.16	34 (7%) 16 13	18, 39, 91, 100	29 (6%)
1	J	468/468 (100%)	0.25	38 (8%) 13 10	18, 39, 91, 100	29 (6%)
1	K	468/468 (100%)	0.22	32 (6%) 18 16	18, 39, 91, 100	29 (6%)
1	L	468/468 (100%)	0.31	32 (6%) 18 16	18, 39, 91, 100	29 (6%)
All	All	5616/5616 (100%)	0.30	522 (9%) 9 7	18, 39, 92, 100	348 (6%)

The worst 5 of 522 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	397	TYR	13.1
1	K	397	TYR	12.7
1	H	402	GLU	12.5
1	B	397	TYR	12.3
1	L	51	GLY	12.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.



## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MPD	G	1489	8/8	0.94	0.35	16.68	16,43,64,74	8
5	MPD	L	1494	8/8	0.92	0.45	15.30	16,43,64,74	8
5	MPD	K	1493	8/8	0.91	0.41	12.92	16,43,64,74	8
5	MPD	F	1488	8/8	0.87	0.43	12.71	16,43,64,74	8
5	MPD	C	1485	8/8	0.85	0.48	11.95	16,43,64,74	8
5	MPD	B	1484	8/8	0.75	0.44	10.37	16,43,64,74	8
5	MPD	H	1490	8/8	0.93	0.41	9.69	16,43,64,74	8
5	MPD	J	1492	8/8	0.92	0.35	9.39	16,43,64,74	8
5	MPD	D	1486	8/8	0.86	0.39	8.51	16,43,64,74	8
5	MPD	I	1491	8/8	0.91	0.32	7.45	16,43,64,74	8
5	MPD	E	1487	8/8	0.91	0.45	5.86	16,43,64,74	8
5	MPD	A	1483	8/8	0.84	0.34	4.11	16,43,64,74	8
3	ADP	F	1476	27/27	0.60	0.51	3.47	20,78,100,100	27
3	ADP	L	1482	27/27	0.67	0.48	3.05	20,78,100,100	27
3	ADP	B	1472	27/27	0.66	0.49	2.96	20,78,100,100	27
3	ADP	I	1479	27/27	0.62	0.50	2.90	20,78,100,100	27
3	ADP	D	1474	27/27	0.65	0.49	2.66	20,78,100,100	27
3	ADP	K	1481	27/27	0.71	0.43	2.24	20,78,100,100	27
3	ADP	C	1473	27/27	0.75	0.35	1.95	20,78,100,100	27
3	ADP	J	1480	27/27	0.84	0.35	1.51	20,78,100,100	27
3	ADP	H	1478	27/27	0.74	0.37	1.43	20,78,100,100	27
3	ADP	E	1475	27/27	0.76	0.35	1.19	20,78,100,100	27
3	ADP	A	1471	27/27	0.69	0.39	1.12	20,78,100,100	27
3	ADP	G	1477	27/27	0.83	0.34	0.95	20,78,100,100	27
4	TL	J	473	1/1	0.93	0.26	-0.47	67,67,67,67	1
4	TL	G	474	1/1	0.96	0.13	-0.49	75,75,75,75	1
4	TL	I	473	1/1	0.86	0.22	-0.55	67,67,67,67	1
4	TL	L	473	1/1	0.93	0.23	-0.68	67,67,67,67	1
4	TL	G	473	1/1	0.96	0.17	-0.77	67,67,67,67	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	D	469	1/1	0.97	0.10	-0.78	34,34,34,34	0
4	TL	A	473	1/1	0.90	0.19	-0.80	67,67,67,67	1
4	TL	I	474	1/1	0.96	0.13	-0.82	75,75,75,75	1
4	TL	H	473	1/1	0.95	0.19	-0.87	67,67,67,67	1
2	MN	G	469	1/1	0.98	0.07	-0.96	34,34,34,34	0
2	MN	J	469	1/1	0.96	0.12	-0.97	34,34,34,34	0
2	MN	H	470	1/1	0.95	0.09	-0.97	41,41,41,41	0
2	MN	J	470	1/1	0.99	0.10	-0.99	41,41,41,41	0
2	MN	I	469	1/1	0.99	0.07	-0.99	34,34,34,34	0
4	TL	C	473	1/1	0.96	0.16	-1.01	67,67,67,67	1
2	MN	L	469	1/1	0.98	0.12	-1.03	34,34,34,34	0
2	MN	K	469	1/1	0.97	0.13	-1.06	34,34,34,34	0
2	MN	H	469	1/1	0.99	0.08	-1.06	34,34,34,34	0
2	MN	E	469	1/1	0.98	0.05	-1.09	34,34,34,34	0
2	MN	C	469	1/1	0.96	0.08	-1.20	34,34,34,34	0
2	MN	B	469	1/1	0.97	0.06	-1.21	34,34,34,34	0
4	TL	D	474	1/1	0.93	0.09	-1.26	75,75,75,75	1
2	MN	F	469	1/1	0.99	0.04	-1.28	34,34,34,34	0
4	TL	F	473	1/1	0.90	0.11	-1.28	67,67,67,67	1
4	TL	E	473	1/1	0.97	0.06	-1.29	67,67,67,67	1
4	TL	K	473	1/1	0.93	0.12	-1.30	67,67,67,67	1
4	TL	L	474	1/1	0.95	0.12	-1.34	75,75,75,75	1
4	TL	D	473	1/1	0.96	0.05	-1.36	67,67,67,67	1
4	TL	E	474	1/1	0.91	0.10	-1.41	75,75,75,75	1
2	MN	A	469	1/1	0.95	0.04	-1.54	34,34,34,34	0
4	TL	B	473	1/1	0.97	0.04	-1.58	67,67,67,67	1
2	MN	A	470	1/1	0.91	0.05	-1.61	41,41,41,41	0
4	TL	J	474	1/1	0.89	0.11	-1.80	75,75,75,75	1
2	MN	C	470	1/1	0.99	0.04	-2.02	41,41,41,41	0
4	TL	K	474	1/1	0.97	0.12	-2.58	75,75,75,75	1
4	TL	A	474	1/1	0.96	0.08	-2.66	75,75,75,75	1
4	TL	B	474	1/1	0.93	0.08	-3.38	75,75,75,75	1
4	TL	F	474	1/1	0.97	0.04	-3.98	75,75,75,75	1
4	TL	H	474	1/1	0.92	0.05	-4.84	75,75,75,75	1
4	TL	C	474	1/1	0.94	0.05	-6.10	75,75,75,75	1
2	MN	D	470	1/1	0.96	0.10	-	41,41,41,41	0
2	MN	F	470	1/1	0.96	0.06	-	41,41,41,41	0
2	MN	G	470	1/1	0.97	0.13	-	41,41,41,41	0
2	MN	L	470	1/1	0.97	0.18	-	41,41,41,41	0
2	MN	E	470	1/1	0.98	0.09	-	41,41,41,41	0
2	MN	B	470	1/1	0.94	0.04	-	41,41,41,41	0
2	MN	I	470	1/1	0.95	0.13	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	K	470	1/1	0.99	0.16	-	41,41,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.